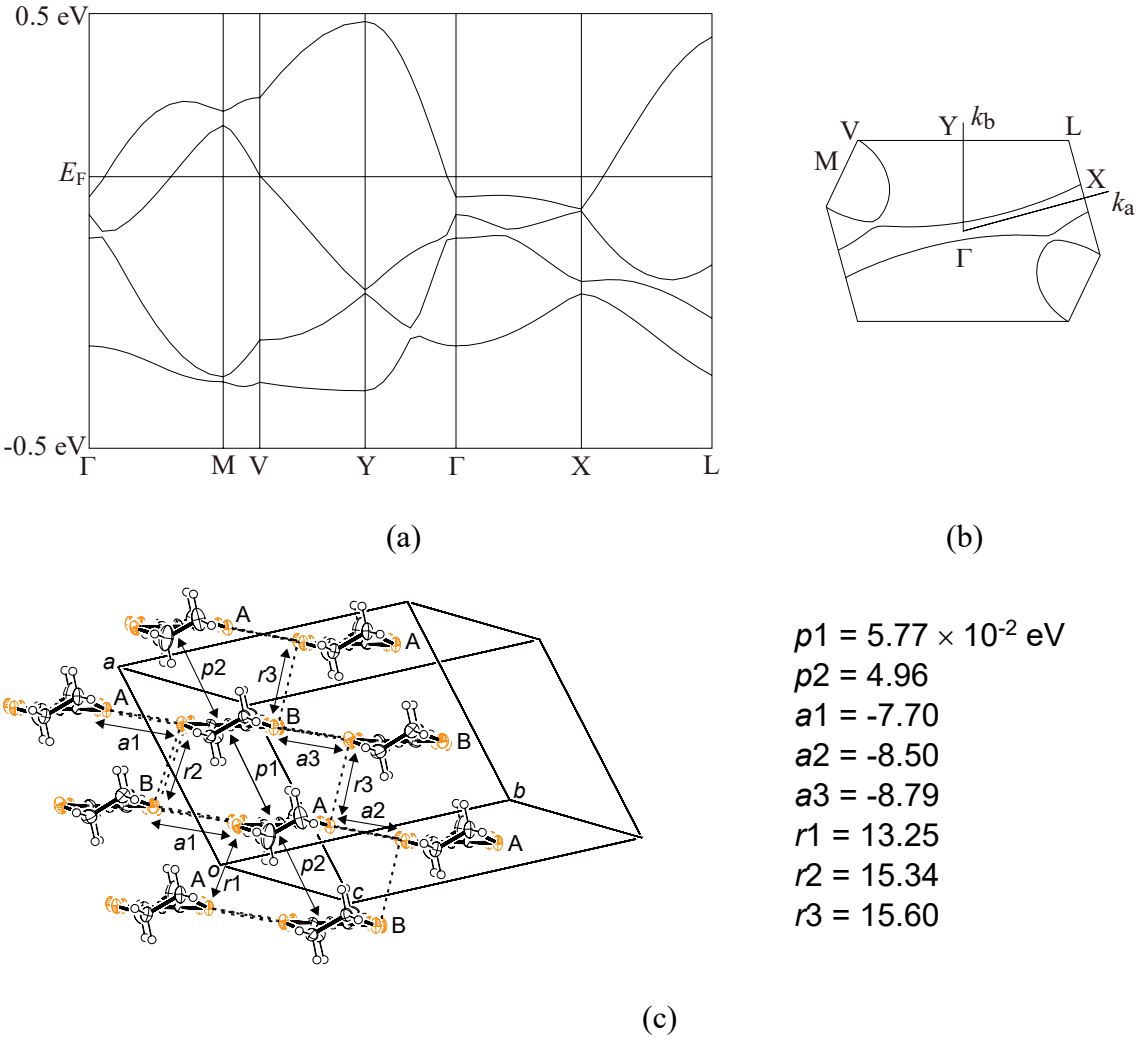
Enantiopure and racemic radical-cation salts of B(mandelate)$_2^-$ and B(2-chloromandelate)$_2^-$ anions with BEDT-TTF

Toby J. Blundell,[a] Kathryn Sneade,[a] Jordan R. Lopez,[a] John D. Wallis,[a] Hiroki Akutsu,[b] Yasuhiro Nakazawa,[b] Simon J. Coles,[c] Claire Wilson[c] and Lee Martin[a*]

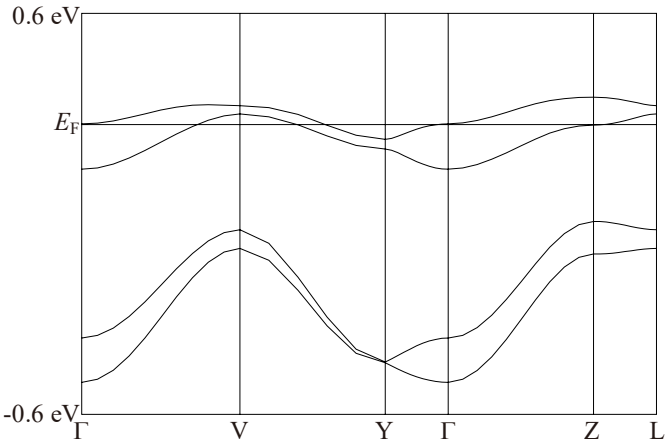


$p1 = 5.77 \times 10^{-2}$ eV
$p2 = 4.96$
$a1 = -7.70$
$a2 = -8.50$
$a3 = -8.79$
$r1 = 13.25$
$r2 = 15.34$
$r3 = 15.60$

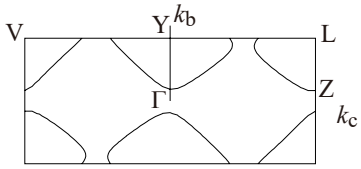
Figure S1. Band dispersions (a), Fermi surfaces (b) and a structure of the donor layers (c) of **I** using a tight binding band structure calculation package on the basis of extended Hückel method written by Prof. Takehiko Mori.[S1-2] Intermolecular interactions are labelled with the transfer integrals listed in (c).

S1) T. Mori, A. Kobayashi, Y. Sasaki, H. Kobayashi, G. Saito, H. Inokuchi, *Bull. Chem. Soc. Jpn.*, 1984, **57**, 627—633.

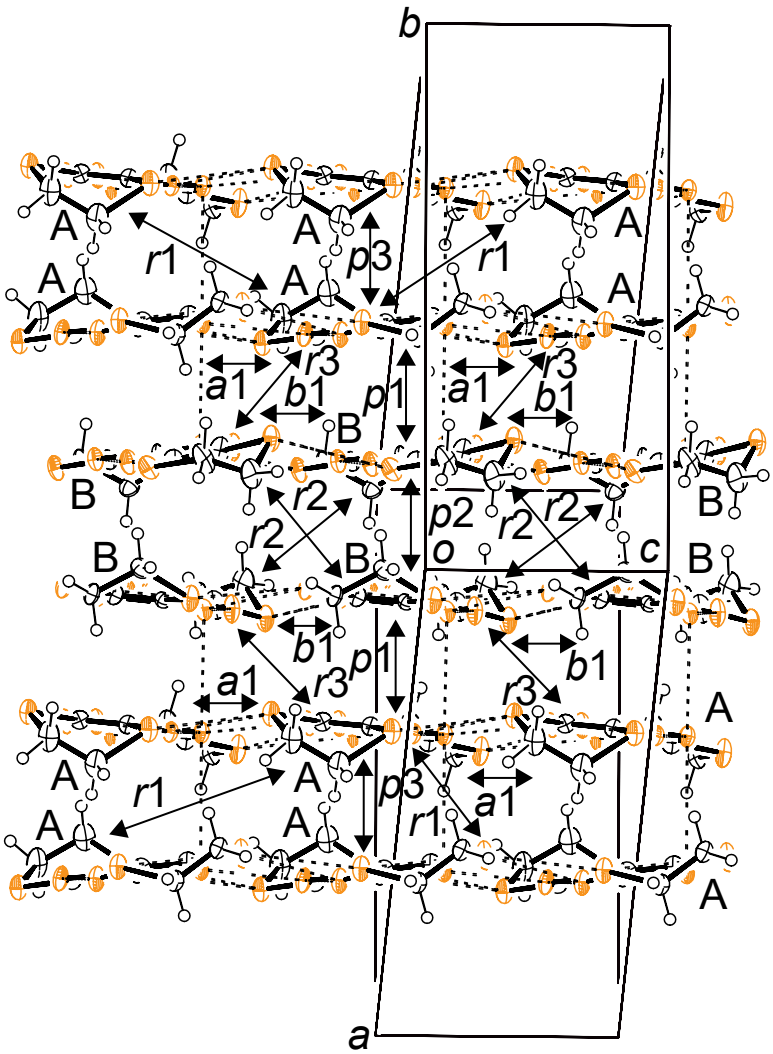
S2) Program Library of Energy Band Calculation for Molecular Conductors, Takehiko Mori, Tokyo Institute of Technology, Japan, http://www.op.titech.ac.jp/lab/mori/lib/program.html.



(a)



(b)



$p1$ = -25.14 × 10^{-2} eV
$p2$ = 7.01
$p3$ = 4.22
$a1$ = 7.59
$b1$ = 4.21
$r1$ = 1.71
$r2$ = 0.23
$r3$ = -6.63

(c)

Figure S2. Band dispersions (a), Fermi surfaces (b) and a structure of the donor layers (c) of **III**.[S1, S2] Intermolecular interactions are labelled with the transfer integrals listed in (c).